Calculus of the Density-of-states in pentacene thin-film transistor

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The first objective of this work consisted of measuring the transfer curve at different temperatures of N-trimethyltriindole from an organic transistor which substrate was made of that material and, analyzing these data, calculate the density of states of N-trimethyltriindole. Unfortunately, it could not be achieved due to the fact that the data collected was not good enough in order to be analyzed. That is the reason why in this work the density of states of the pentacene is calculated from the electrical characteristics of a thin-film transistor measured at different temperatures.

Keywords: Thin-film transistor, Density of states, Organic semiconductor, Pentacene.

I. INTRODUCTION

A transistor is an electronic device used to amplify or switch electronic signals and electrical power. It consists of a substrate, a gate, a source and a drain. The gate is made of an oxide (SiO_2) which thickness equals 150 nm **[1]**, and the substrate is a semiconductor. In the case of an organic thin-film transistor, it corresponds to an organic material. This kind of transistors has several benefits. Apart from being environmentally friendly, they are cheaper than the ones made of inorganic materials and their fabrication process is much easier due to the fact that they can be done at room temperature. Nowadays, they are used in some sensors, flexible displays and memory devices.

FIG.1.(Color online) Example of application: flexible display by the Korean company LG electronics. It is a 18-inch (about 46cm) rollable display, which was announced on January at Las Vegas. Credit of the photo: LG Display [**2**]

In the research area, knowing the density of states (DOS) of a semiconductor can be very useful in order to provide a wide knowledge of the material and thin-film transistors are especially useful devices to study precisely the DOS of semiconducting layers. The calculus of the DOS is based on the analysis of the activation energy **[2]**. This reduces when the gate voltage is increased because the Fermi level approaches the conducting edge (LUMO). The DOS is related to the variation of the activation energy with respect to de gate voltage.

II. THEORETICAL BACKGROUND

Organic thin-film transistors (OTFTs) based on semiconducting small molecules have reached the electrical performance of amorphous silicon, the benchmark for organic electronic devices. However, the development of these devices may be more impressive if the knowledge of the materials is improved, i.e. if a characterization of the charge transport is done. If organic transistors are thought in terms of conduction and valence bands, as in semiconductors, these concepts correspond to the Highest Occupied and Lowest Unoccupied Molecular Orbital (HOMO and LUMO) levels of organic semiconductors. In small-molecule semiconductors it is generally accepted that electrical conduction takes place in these extended state transport levels (HOMO level for holes and LUMO for electrons) where charge carriers are activated from localized states. A crucial feature for studying charge transport in these materials is the determination of the density-of-states (DOS) in the gap of the semiconductor, and the model used is called multiple trapping and thermal release model (MTR). Thin-film transistors are widely used devices to know about the DOS of semiconducting layers

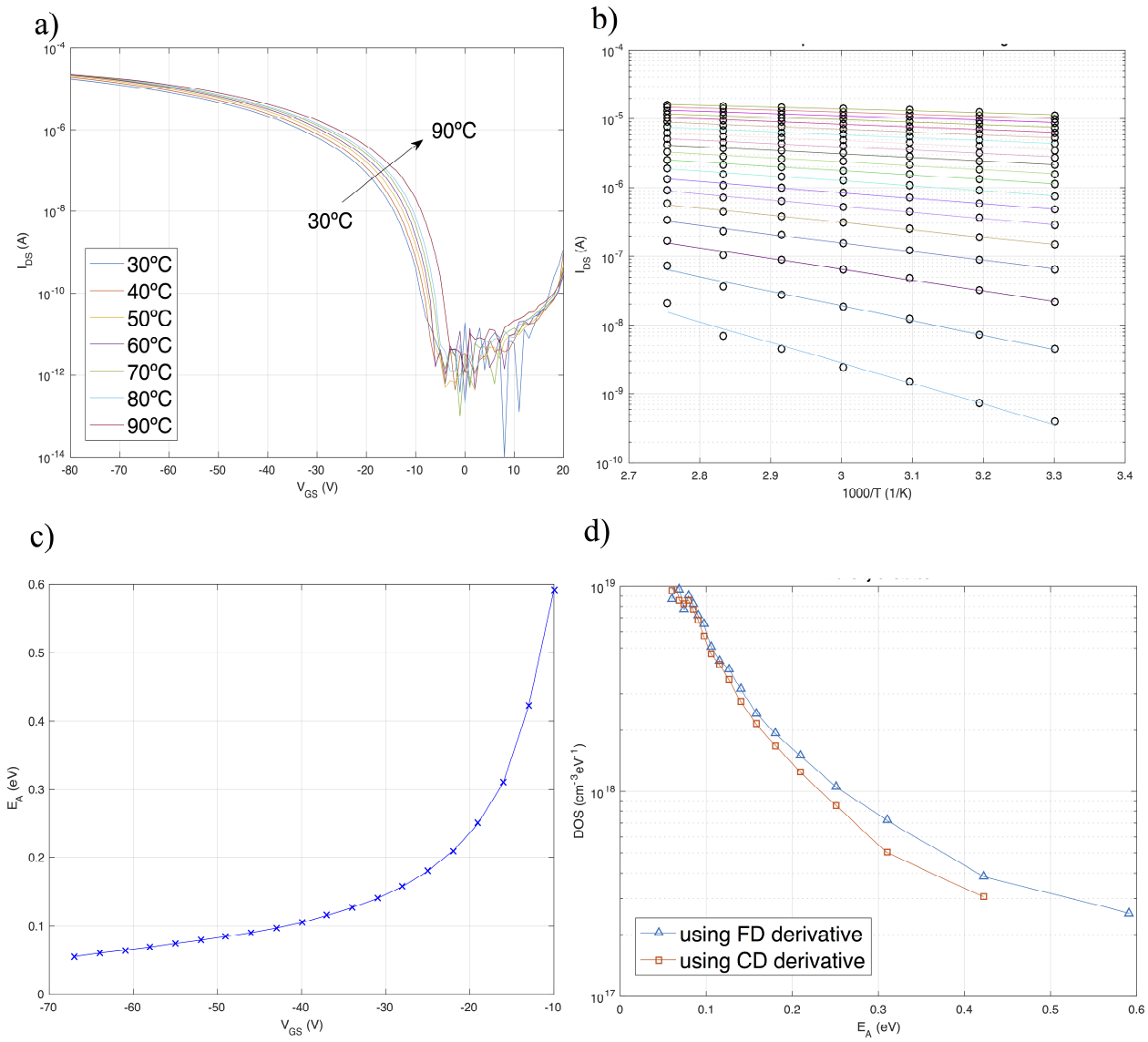

FIG. 2. a) Transfer characteristics of the pentacene OTFT measured at different temperatures (from 30ºC to 90ºC) in vacuum while cooling down the Device. The V_{DS} voltage was -10V for all these measurements. b) This plot shows the drain current for different gate voltages. The lines are exponential fits to calculate the activation energy of the channel conductivity. c) Activation energy of the channel conductivity as a function of V_{GS} for the transfer characteristics. d) Density-of-states in the gap of pentacene calculated from the derivative of the activation energy of the channel conductivity.

because the Fermi level can be shifted through the distribution of localized states by means of the gate voltage. To achieve this knowledge, a method based on the analysis of the thermal activation energy of the channel conductance is used. More precisely, the activation energy reduces when increasing the gate voltage as the Fermi level moves towards the band edge. The Fermi level shifts when increasing the gate voltage at a rate which is influenced by the density of localized states in the gap. This effect can be explained as follows: when the voltage applied equals the threshold voltage (which is the voltage inducing flat band conditions), there is no induced charge in the organic film. However, when the voltage applied is greater than the threshold, holes are injected into the organic film channel from the grounded source and drain electrodes to screen the gate negative charge. These holes populate the states of the HOMO band; consequently, the Fermi level shifts closer to the molecular energy level. Assuming then that charge density within the channel is dominated by trapped carriers; DOS can be related to the derivative of the activation energy with respect to gate bias.

III. MEASUREMENTS

The first objective of this project was to calculate the DOS from the transfer characteristic of an organic transistor made of N-trimethyltriindole. In order to get the transfer curve, the transistor was settled in a cryostat where the drain, the source and the gate were connected. Those were also connected to SourceMeter controlled with a computer so the source-drain current could be measured at different gate voltages in order to get the desired characteristic. This process had to be repeated at different temperatures (from 300K to 390K). A programmable temperature controlled was used so that the transistor could be heated.

The idea was to treat these data to calculate the DOS but the results obtained from the measurements were not good enough.

The same measurements were done with a transistor which source consisted of BOBTP but the results were not good either. It is thought that the cause of this is the fact that it arrives a moment when the Fermi level and the LUMO level aligned each other which causes the non-variation of the transfer characteristic when the temperature is increased.

Due to these problems, data from the transfer curve at different temperatures of a pentacene organic transistor was analyzed to calculate the DOS of this material.

IV. CALCULUS OF THE DOS

The DOS of the pentacene was calculated in several steps. First of all, the transfer characteristics at different temperatures were represented in the same plot. As it can be seen in Figure 2(a), the shape of the curve is always the same but the current increases with temperature. Then, the values of the drain-source current for the different temperatures at a given gate voltage were selected. This was done for different gate voltages.

The next step was to plot the current with respect to (1000/T) using a logarithmic scale (Figure 2(b)). The drain source current is given by (1) **[3]**, where E_A is the activation energy, T is the temperature, K is the Boltzmann constant and I_{D0} is a constant.

A straight line was fitted to this data so that the activation energy could be calculated from the slope as it can be seen in (2).

$$I_{DS} = I_{D0} e^{-\frac{E_A}{KT}} \tag{1}$$

$$\log(I_{DS}) = -\frac{E_A}{KT} + \log(I_{D0}) = a\frac{1}{T} + b \tag{2}$$

After that, the activation energy was represented with respect to the gate voltage (Figure 2(c)). This is used to calculate the DOS from (3), where t is the thickness of the carriers channel (10 nm), q is the electron charge and C is the oxide capacity and is calculated from (4) **[4].**

$$N(E) = \frac{C}{q \cdot t}\left(\frac{\partial E_A}{\partial V_{GS}}\right)^{-1} \tag{3}$$

$$C = \frac{\varepsilon_r \varepsilon_0}{d} \tag{4}$$

In (4), d corresponds to the thickness of the oxide, ε_r is its relative permeability (in the case of the SiO_2 it is 3,9) and ε_0 is the vacuum permeability.

Finally, the DOS was represented with respect to the activation energy, as it is shown in Figure 2(d). In order to do so, two different numeric derivative methods have been used: CD (central difference) and FD (forward difference).

As can be seen in Figure 2(d), the DOS exponentially increases up to $10^{19}\ cm^{-3}$ close to the valence band edge.

V. CONCLUSIONS

The calculus carried out in this work contributes to a better understanding of the characteristics of the pentacene as the activation energy of the channel conductance as a function of the gate voltage gives valuable information of the density of states in the active layer. And not only for pentacene but this method could be repeated measuring other OTFTs made of different substrates such as α-sexithiophene, poly-3-hexylthiophene or *n*-channel benzobisimidazobenzophenanthroline, in order to obtain the density of states of different organic materials.

Obtaining the DOS of different materials can be very useful as it appears in many areas of physics, and helps to explain a number of quantum mechanical phenomena. For example **[5]**, in order to optimize the performance of organic electronic devices, a minimization of the charge carrier injection barriers and of the extraction losses at interfaces between organic semiconductors and metallic electrodes is needed. In order to do this, there exists an electrostatic model capable of reproducing the alignment between the electrode Fermi energy and the transport states in the organic semiconductor, in which the density of states is needed.

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